

Express The Rate Of The Reaction In Terms Of The Rate Of Concentration Change For Each Of The Three Species

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Understanding how to express the rate of a chemical reaction in terms of the concentration changes of its reactants and products is fundamental in chemical kinetics. This approach allows chemists to quantify how quickly a reaction proceeds and how the concentrations of various species evolve over time. Specifically, for reactions involving three species—typically two reactants and one product—the rate can be expressed in relation to the rate of change of each species' concentration. This method facilitates the comparison of the relative consumption and production rates, providing insight into the reaction mechanism and the dynamics of the process.

In this comprehensive guide, we will explore how to derive and interpret the rate expressions for reactions involving three species. We will discuss the fundamental principles, the role of stoichiometry, and how to formulate rate expressions that accurately describe the reaction kinetics. Whether you're a student studying chemical kinetics or a researcher analyzing reaction mechanisms, this guide aims to clarify the methodology for expressing reaction rates in terms of concentration changes.

Understanding Reaction Rates and Concentration Changes

What Is a Reaction Rate?

The reaction rate is a measure of how quickly reactants are converted into products over time. It is typically expressed as the change in concentration of a species per unit time:

- Rate of consumption of reactants
- Rate of formation of products

Mathematically, for a generic reaction:



the rate can be expressed as:

$$\text{Rate} = -\frac{1}{a} \frac{d[A]}{dt} = -\frac{1}{b} \frac{d[B]}{dt} = \frac{1}{c} \frac{d[C]}{dt}$$

The negative sign indicates consumption of reactants, while the positive indicates formation of products.

Why Express Rate in Terms of Concentration Changes?

Expressing the reaction rate in terms of concentration changes provides:

- A quantitative measure of how concentrations evolve over time
- A means to compare the rates at which different species are consumed or produced
- Insight into the reaction mechanism and rate-determining steps
- A foundation for deriving rate laws and kinetic models

General Approach to Expressing the Rate for Reactions with Three Species

Typical Reaction Framework

Consider a generic reaction involving three species:



where:

- A , B are reactants,
- C is the product,
- a , b , and c are their respective stoichiometric coefficients.

In many cases, reactions might involve two reactants converting into a product, or more complex schemes involving intermediates. The key is to relate the rate to the concentration changes of each species involved.

Formulating the Rate Expression

To express the rate in terms of the concentration changes of each species, follow these steps:

1. Identify the stoichiometric coefficients for all species involved.
2. Define the rate of reaction (also called the average rate) based on a specific species, usually a reactant or the primary species of interest.
3. Express the rate of the reaction in terms of the concentration change of each species, scaled by the inverse of their stoichiometric coefficients.

4. Ensure consistency across all species, maintaining the sign conventions (positive for formation, negative for consumption).

General rate expressions:

- For a reaction $aA + bB \rightarrow cC$,

$$\text{Rate} = -\frac{1}{a} \frac{d[A]}{dt} = -\frac{1}{b} \frac{d[B]}{dt} = \frac{1}{c} \frac{d[C]}{dt}$$

This set of equalities ensures the rate is consistently expressed in terms of each species' concentration change.

Expressing the Reaction Rate in Terms of Concentration Change for Each Species

Step-by-Step Derivation

Let's consider a specific example to clarify the process:

Example Reaction:



Step 1: Identify stoichiometric coefficients:

- $a = 1$ for A ,

- $(b = 2)$ for (B) ,
- $(c = 1)$ for (C) .

Step 2: Write the rate of the reaction in terms of each species:

$$\text{Rate} = -\frac{1}{1} \frac{d[A]}{dt} = -\frac{1}{2} \frac{d[B]}{dt} = \frac{d[C]}{dt}$$

Step 3: Express the rate of reaction as a common quantity, for example, based on the consumption of (A) :

$$\text{Rate} = -\frac{d[A]}{dt}$$

Step 4: Express the concentration change of (B) and (C) in terms of this rate:

$$-\frac{1}{2} \frac{d[B]}{dt} = -\frac{d[A]}{dt} \Rightarrow \frac{d[B]}{dt} = 2 \frac{d[A]}{dt}$$

$$\frac{d[C]}{dt} = \frac{d[A]}{dt}$$

Step 5: Final expressions:

$$\boxed{\begin{aligned} \text{Rate} &= -\frac{d[A]}{dt} \\ \text{Rate} &= -\frac{1}{2} \frac{d[B]}{dt} \\ \text{Rate} &= \frac{d[C]}{dt} \end{aligned}}$$

\]

Generalized Formula for Reactions with Three Species

For a reaction involving three species:



the rate can be expressed as:

$$\boxed{\text{Rate} = -\frac{1}{a} \frac{d[A]}{dt} = -\frac{1}{b} \frac{d[B]}{dt} = \frac{1}{c} \frac{d[C]}{dt}}$$

This set of equations allows the calculation of the rate based on the concentration change of any species involved, provided the stoichiometric coefficients are known.

Implications for Reaction Mechanism and Kinetics

Understanding Reaction Dynamics

Expressing the reaction rate in terms of concentration changes helps in:

- Determining the order of the reaction with respect to each species

- Identifying the rate-determining step in complex mechanisms
- Designing experiments to measure reaction rates and validate kinetic models

Determining Rate Laws

The rate expressions form the basis for deriving rate laws, which are empirical or semi-empirical formulas describing how the rate depends on concentrations:

$$\text{Rate} = k [A]^m [B]^n$$

where k is the rate constant, and (m, n) are reaction orders.

By analyzing concentration changes over time, one can determine these parameters experimentally.

Practical Applications and Examples

Example 1: Simple Reaction with Three Species

Consider the reaction:



The rate expressions are:

$$\text{Rate} = -\frac{1}{2} \frac{d[A]}{dt} = -\frac{d[B]}{dt} = \frac{d[C]}{dt}$$

If experimental data shows that $\frac{d[A]}{dt}$ is -0.02 , $\text{mol/L}\cdot\text{s}$, then:

- Rate of reaction: 0.02 , $\text{mol/L}\cdot\text{s}$
- $\frac{d[B]}{dt} = 2 \times 0.02 = 0.04$, $\text{mol/L}\cdot\text{s}$
- $\frac{d[C]}{dt} = 0.02$, $\text{mol/L}\cdot\text{s}$

This approach allows chemists to track how each species changes and interpret the reaction's kinetics.

Example 2: Complex Reaction Scheme

In more complex reactions involving intermediates, the same principles apply, but additional steps are involved in relating the concentration changes of each species to the overall reaction rate. Steady-state approximations or integrated rate laws are used to analyze such systems.

Summary and Key Takeaways

- Reaction rates can be expressed in terms of the rate of change of concentration for each species involved in the reaction.
- The basic

Frequently Asked Questions

What is the general expression for the rate of a reaction in terms of the concentration change of each species?

The rate of a reaction can be expressed as the negative or positive change in concentration of each species over time, divided by its stoichiometric coefficient, for example: Rate = $-(1/a) (d[A]/dt) = -(1/b) (d[B]/dt) = (1/c) (d[C]/dt)$, where a, b, c are the stoichiometric coefficients.

How do you express the rate of reaction using the concentration change of a reactant?

The rate of reaction is expressed as the negative of the rate of change of reactant concentration over time divided by its stoichiometric coefficient: Rate = $-(1/a) (d[A]/dt)$.

How is the rate expressed in terms of the product concentration change?

For a product, the rate of reaction is given by the positive rate of change of its concentration divided by its stoichiometric coefficient: Rate = $(1/c) (d[C]/dt)$.

Why is the concentration change of reactants negative in the rate expression?

Because reactant concentrations decrease over time during the reaction, their rate of change is negative, so the expression includes a negative sign to give a positive rate of reaction.

Can the same rate expression be written for all three species in a reaction?

Yes, the rate can be expressed in terms of the concentration change of any species, but each expression includes the respective stoichiometric coefficient to ensure consistency across the reaction.

How do you determine the rate expression from experimental data involving concentration changes?

You measure the rate of change of concentration of each species over time, then divide by their respective stoichiometric coefficients, ensuring all expressions are consistent and yield the same reaction rate.

What does the sign convention in the rate expressions indicate?

A negative sign indicates the concentration of reactants decreases over time, while a positive sign indicates the concentration of products increases during the reaction.

How do the rate expressions relate to the overall reaction stoichiometry?

The rate expressions are directly related to the stoichiometric coefficients; dividing the concentration change rate by these coefficients standardizes the rate across different species in the balanced equation.

Why is it important to express the reaction rate in terms of concentration changes for each species?

Because it allows for a consistent and quantitative understanding of the reaction kinetics, enabling calculation of the rate and understanding how each species influences the overall reaction rate.

Additional Resources

Express The Rate Of The Reaction In Terms Of The Rate Of Concentration Change For Each Of The Three Species

Introduction

In chemical kinetics, understanding how the concentration of reactants and products change over time is fundamental to elucidating reaction mechanisms, optimizing industrial processes, and predicting reaction behavior under various conditions. Central to this understanding is the concept of the reaction rate, a measure that quantifies how quickly reactants are converted into products. When dealing with reactions involving multiple species, especially elementary reactions with multiple reactants and products, expressing the rate of the reaction in terms of the rate of concentration change of each individual species becomes crucial.

This article aims to develop a comprehensive framework for relating the overall reaction rate to the rates of concentration change of each species involved, with particular emphasis on reactions involving three species. We will explore the mathematical formulation, discuss the

concept of reaction orders, and elucidate how stoichiometry influences the expressions linking individual species' rates to the overall reaction rate.

Fundamental Concepts in Reaction Rate Expressions

The Reaction Rate and Its Definition

The reaction rate is formally defined as the change in concentration of a species per unit time:

$$\text{Rate of species } i = -\frac{1}{\nu_i} \frac{d[C_i]}{dt}$$

where:

- $[C_i]$ is the concentration of species i ,
- ν_i is the stoichiometric coefficient of species i in the balanced chemical equation.

The negative sign indicates that for reactants, concentration decreases over time, whereas for products, concentration increases.

General Kinetic Expression

For a generic chemical reaction:



the reaction rate (often denoted as r) is related to the rate of change of concentration of each species via:

$$r = \frac{1}{\nu_i} \frac{d[C_i]}{dt}$$

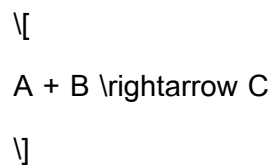
with the convention that:

- $(r > 0)$,
- $(d[C_i]/dt)$ is negative for reactants (decreasing),
- $(d[C_i]/dt)$ is positive for products (increasing).

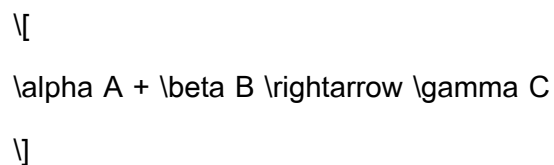
Expressing Reaction Rate in Terms of Concentration Changes for Three-Species Reactions

Example: A Three-Species Elementary Reaction

Consider an elementary reaction involving three species:



or more generally,



where (α, β, γ) are stoichiometric coefficients.

Reaction Rate Definition for Multi-Species Reactions

The reaction rate r is connected to the concentration changes via:

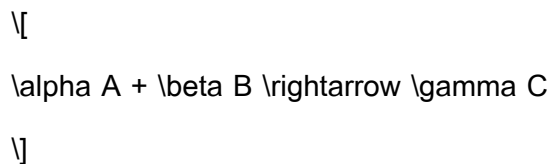
$$r = -\frac{1}{\alpha} \frac{d[A]}{dt} = -\frac{1}{\beta} \frac{d[B]}{dt} = \frac{1}{\gamma} \frac{d[C]}{dt}$$

This set of equalities signifies that the reaction rate is consistent across all species, but scaled according to their stoichiometry.

Deriving Expressions for Each Species' Concentration Rate

General Formulation

For a general reaction involving three species (A, B, C):



the reaction rate r can be expressed as:

$$r = -\frac{1}{\alpha} \frac{d[A]}{dt} = -\frac{1}{\beta} \frac{d[B]}{dt} = \frac{1}{\gamma} \frac{d[C]}{dt}$$

Alternatively, rearranged to express the rate of concentration change of each species:

$$\frac{d[A]}{dt} = -\alpha r$$

]

$$\frac{d[B]}{dt} = -\beta r$$

]

$$\frac{d[C]}{dt} = \gamma r$$

]

This relationship forms the core of how the overall reaction rate relates to individual concentration changes.

Expressing The Rate of Reaction in Terms of Concentration Changes

The Rate Law and Reaction Order

The rate law for a reaction involving three species typically takes the form:

$$r = k [A]^m [B]^n [C]^p$$

]

where:

- k is the rate constant,
- (m, n, p) are the reaction orders with respect to (A, B, C) , respectively.

The reaction order with respect to each species indicates how sensitive the rate is to the change in that species' concentration.

Formal expressions

Using the rate law, the individual rates of change are:

$$\frac{d[A]}{dt} = -\alpha r = -\alpha k [A]^m [B]^n [C]^p$$

$$\frac{d[B]}{dt} = -\beta r = -\beta k [A]^m [B]^n [C]^p$$

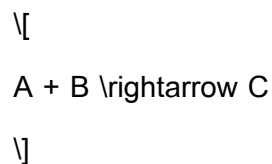
$$\frac{d[C]}{dt} = \gamma r = \gamma k [A]^m [B]^n [C]^p$$

Note: These expressions assume elementary kinetics and that the rate law matches the reaction's molecularity.

Practical Applications and Examples

Example 1: A Simple Three-Species Reaction

Suppose we have the reaction:



with rate law:

$$r = k [A][B]$$

The concentration change rates are:

$$\frac{d[A]}{dt} = -k [A][B]$$

$$\frac{d[B]}{dt} = -k [A][B]$$

$$\frac{d[C]}{dt} = +k [A][B]$$

This straightforward relation illustrates that the reaction rate is directly proportional to the product of the reactants' concentrations.

Example 2: A Reversible Reaction

Consider:



with forward and reverse rate constants k_f and k_r . The net rate is:

$$r_{\text{net}} = k_f [A][B] - k_r [C]$$

\]

Expressing concentration changes:

\[

$$\frac{d[A]}{dt} = - \alpha r_{\text{net}}$$

\]

\[

$$\frac{d[B]}{dt} = - \beta r_{\text{net}}$$

\]

\[

$$\frac{d[C]}{dt} = \gamma r_{\text{net}}$$

\]

This dynamic model captures the equilibrium behavior and how individual species' concentrations evolve over time.

Influence of Stoichiometry and Reaction Mechanisms

The stoichiometric coefficients are critical in translating between the reaction rate and species concentration changes. For complex reactions with multiple steps and intermediates, the overall rate expression becomes a sum of elementary steps, each with its own rate law, and the overall relationship involves considering the rate-determining step.

In cases where the reaction proceeds via a mechanism involving three species, often with complex stoichiometry, the following considerations are essential:

- Reaction order determination: experimentally or theoretically derived, affecting how concentration changes relate to the overall rate.

- Stoichiometric coefficients: influence the proportionality factors between species' concentration changes and the reaction rate.
- Steady-state or pre-equilibrium assumptions: may simplify the expressions, especially in complex mechanisms.

Limitations and Considerations

While the relationships outlined provide a robust framework, several factors can complicate the direct linkage:

- Non-elementary reactions: where the rate law does not correspond directly to molecularity.
- Involvement of catalysts: altering apparent reaction orders.
- Reaction conditions: temperature, pressure, and solvent effects impacting rate constants.
- Complex mechanisms: involving multiple steps, intermediates, and reversible reactions.

Understanding these limitations is essential for accurate kinetic modeling.

Conclusion

Expressing the reaction rate in terms of the rate of concentration change for each species provides a powerful tool for analyzing and predicting reaction behavior. For reactions involving three species, the fundamental relationships hinge on the stoichiometry and the reaction order, encapsulated in the rate law. The core expressions:

$$\left[\begin{aligned} \frac{d[A]}{dt} &= -\alpha r, \quad \frac{d[B]}{dt} = -\beta r, \quad \frac{d[C]}{dt} = \gamma r \end{aligned} \right]$$

serve as the foundation for kinetic analysis. These relationships enable chemists and engineers to translate observed concentration changes into an understanding of the overall reaction dynamics, facilitate the determination of rate constants, and optimize reaction conditions for desired outcomes.

In advancing the field, ongoing research continues to refine these models, especially for complex, multi-step reactions, ensuring that the expressions for reaction rates remain both accurate and practically useful across diverse chemical systems.

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